### Appendix A

OU 10-08 External Review Team Letter Report and Recommendations

#### EXTERNAL REVIEW TEAM

Edgar Berkey, Ph.D., Chair R.L. Bassett, Ph.D. Michael Kavanaugh, Ph.D. Peter Wierenga, Ph.D.

August 14, 2004

Idaho National Engineering and Environmental Laboratory Bechtel BWXT Idaho, LLC P. O. Box 1625 Idaho Falls, ID 83415 Attn: Mr. Erick R. Neher

Subject: WAG 10 Site-Wide Groundwater Model

Dear Mr. Neher:

As requested, this letter presents the final results of an independent on-site review of your plans to develop a Waste Area Group (WAG) 10 site-wide groundwater model at the Idaho National Engineering and Environmental Laboratory (INEEL). We understand such a model is being developed as a project task within the Balance of INEEL Cleanup group at the INEEL to meet regulatory requirements for final remediation of the site.

An External Review Team (ERT) consisting of Drs. Edgar Berkey (chair), R.L. Bassett, Michael Kavanaugh, and Peter Wierenga conducted the on-site review during the period May 19-21, 2004. These individuals are former members of the Groundwater/Vadose Zone Expert Panel at the Hanford site, a three-years plus undertaking within the Integration Project at Hanford that encountered many of the same issues being faced by the current WAG 10 effort. In addition, members of the ERT are also recognized as generally knowledgeable on groundwater issues within the DOE complex. Attachment A provides brief bio-sketches of the ERT members. For the record, a draft of this letter was submitted for review as agreed on June 7, 2004.

In organizing this review, it was recognized by all that the effort to develop a site-wide groundwater model at the INEEL was still at an early stage. A multi-disciplinary team of INEEL staff with the needed modeling skills and related technical experience has only recently been pulled together to begin a concerted effort on the project. A draft Work Plan that will be used to guide development of the eventual groundwater model is still being defined. Nevertheless, it was deemed an excellent time to hold an early external review of the WAG 10 modeling plans with the expectation that the final Work Plan would be improved by the ERT's comments.

#### **EXECUTIVE SUMMARY**

Current plans to develop a WAG 10 site-wide groundwater model at the INEEL were reviewed by an independent External Review Team (ERT). While development of such a model is a requirement to complete the RI/FS for WAG 10, the ERT concluded that the

Mr. Erick R. Neher August 14, 2004 Page 2 of 23

model can also become a valuable tool for future remedial action decision-making, stakeholder communications, and long-term stewardship of the site. The ERT strongly supports development of the model and believes that the general approach being taken by the development team is both technically and administratively sound. The ERT found that the team is well aware of the data shortcomings and modeling challenges that must be overcome and seems well staffed and organized to address them. The existing draft Work Plan was deemed to be a good start, and the ERT made a number of suggestions for the final Work Plan, including improving how sub-surface contaminant transport is described, defining what transport models will be used, and benefiting from relevant lessons learned from Hanford. However, for the effort to be fully successful, the ERT believes that continued support will likely be required from high-level champions on both the contractor and DOE-ID side of the house given that previous practice and current site culture runs somewhat counter to accepting a site-wide model.

#### **OBJECTIVE OF THE REVIEW**

The objective of this review was to evaluate the INEEL's current plans for development of a WAG 10 site-wide groundwater model, make observations and draw conclusions regarding the proposed approach, and provide recommendations intended to improve the approach.

#### RELEVANT BACKGROUND

At the INEEL, WAG 10 Operable Unit (OU) 10-08 has been defined to encompass the entire site for the purpose of carrying out a comprehensive site-wide evaluation of environmental impacts from all INEEL operations on the underlying Snake River Plain Aquifer. Thus, the Remedial Investigation/Feasibility Study (RI/FS) required for OU 10-08 must investigate potential cumulative impacts to groundwater from all site operations.

Previous efforts to evaluate groundwater impacts at the INEEL have been performed only on a WAG-specific basis and have not considered cumulative impacts. Therefore, in order to meet the regulatory requirements applying to WAG 10 in support of future site remedial and closure decisions, it is well accepted that a site-wide aquifer flow and contaminant transport numerical model must be developed for the INEEL.

The task to develop a site-wide groundwater fate and transport model has been assigned to the Balance of INEEL Cleanup group at the INEEL. The effort to develop the technical and functional requirements and specifications for the model and to prepare a Work Plan for this task began during the second quarter of FY2004. Because in many respects this work is breaking new ground at the INEEL, it was thought beneficial, even at this early stage, to obtain an external, independent review of the proposed approach.

Mr. Erick R. Neher August 14, 2004 Page 3 of 23

#### REVIEW PROCEDURE

Each member of the ERT was sent a packet of relevant documents to review prior to attending an on-site meeting at the INEEL on May 19-21, 2004. These documents are referenced at the end of this letter in the priority order indicated by the staff. In general, the documents provide background information and a current status report on the plans to develop a site-wide groundwater model under WAG 10, including summary information on existing knowledge of subsurface groundwater flow and existing contamination beneath the INEEL. The present draft of the Work Plan for the modeling effort was also included in the packet.

On May 19, 2004, the ERT was given a series of briefings by the INEEL WAG 10 groundwater modeling team. This is the group of individuals assembled under the leadership of Mr. Tom Wood to carry out the effort. Attachment B to this letter presents the agenda for these briefings. To guide the overall review, Mr. Erick Neher provided a set of seven guiding questions to the ERT with the expectation they would serve as the basis for the review. Although the questions were not intended to limit the ERT's comments, they were thoughtfully prepared, and the ERT chose to respond to each of them.

The ERT very much appreciated that the presenters at the May 19 review meeting were generally well prepared and had useful briefing slides. This contributed to an excellent exchange of information and highly interactive discussions providing opportunities for many substantive interactions between the ERT and the modeling team that were essential to the review.

On May 20, 2004, the ERT provided an outbrief to the WAG 10 modeling team on its preliminary set of observations, conclusions, and recommendations resulting from the review. On May 21 2004, the Review Team provided a similar but less detailed outbrief to Lisa Green and Katie Hain of DOE-ID.

#### OVERALL OBSERVATIONS AND CONCLUSIONS

1. Development of a site-wide groundwater model for the INEEL that includes both fate and transport of contaminants is required to complete the RI/FS for the WAG 10 OU 10-8. Such a model will also provide the INEEL with several additional important capabilities, as it has the potential to become a very significant new tool for remedial action decision-making, stakeholder communications, and long-term stewardship of the site.

Mr. Erick R. Neher August 14, 2004 Page 4 of 23

The ERT fully endorses the effort underway to develop and implement a comprehensive site-wide fate and transport groundwater model at the INEEL. The benefits of having such a model available are abundantly clear and have been well identified by the WAG 10 modeling group both in their documents and during the review meeting. Although the development task to produce the model will be challenging, the ERT believes that the task is doable with a reasonable effort and investment. Moreover, the existence of a site-wide groundwater model will yield significant dividends by allowing more confident and defensible predictions of the cumulative impacts of INEEL operations on the underlying Snake River Plain Aquifer. This capability will be essential to promoting and securing stakeholder concurrence, as well as establishing future new missions at the INEEL.

2. The general approach being taken by the WAG 10 modeling group to develop a site-wide groundwater model is good, both technically and administratively.

Development of a site-wide groundwater model represents a significant cultural departure from past practice at the INEEL. Previously, groundwater models were developed only on a WAG-specific basis, and there was no ability to determine cumulative risks from site operations with much confidence. The WAG 10 modeling effort recognizes that it must build on and be compatible with previous modeling efforts on site. Consequently, the ERT is pleased that the modeling group formed for WAG 10 includes strong technical representatives from other WAGs. We also support the stated desire to involve regulators and other stakeholders on a continuing basis in the effort and to incorporate their input as appropriate. Periodic meetings are planned with all the participants to discuss and report on progress and to identify any necessary changes in direction that are required.

The ERT believes that operating in this fashion will increase the likelihood that the WAG 10 modeling group will produce a useful model. We think the group consists of technical and management personnel having the necessary technical background and experience to succeed. However, full confidence in the utility of the WAG 10 modeling effort will ultimately depend principally on the quality of the underlying databases that are incorporated, the rigorous procedures that are used in calibration, and the ability to identify and reduce the uncertainty of predictions. The technical approach being used by the WAG 10 modeling group is sensitive to these issues and includes plans to address each of them. The ERT believes that the plans developed to date are good. Future reviews would be desirable to assure that the effort remains on track.

3. Because development of a site-wide groundwater model at the INEEL runs counter to previous practice and site culture, there are likely to be a variety of internal and external issues that must be addressed with time as disparate views and local cultures are integrated. Overcoming these challenges to produce an integrated groundwater model and reap the benefits of the results will likely

4

Mr. Erick R. Neher August 14, 2004 Page 5 of 23

### require high-level champions for the WAG 10 modeling efforts on both the contractor side and the DOE-ID side.

The WAG 10 modeling effort is essentially an effort to produce an integrated view of the groundwater situation at the INEEL. Since development of an integrated view has not previously been accomplished, the ERT expects that inevitably there will be challenges to be overcome arising from differences in local views, culture, or past practices regarding individual WAGs. It is critical to the success of the WAG 10 modeling mission that such obstacles not become showstoppers.

Based on our experience over several years with groundwater modeling efforts at Hanford and at other locations, the ERT is convinced of the technical and economic benefits associated with integrating groundwater-modeling efforts on a site-wide basis at DOE sites. Integration can leverage and extend budgets. It can also assist in filling data gaps, for example, as individual projects at the WAG level coordinate fieldwork to provide data that also benefits the modeling effort. Such "integration economies" were seen at Hanford. However, the ERT also recognizes that integration did not take place at Hanford, and will not take place at the INEEL, without considerable support from upper management on both the contractor side and the DOE side. The WAG 10 effort clearly has strong local management support. We would hope that other high-level champions also emerge over time at the INEEL to support the WAG 10 modeling efforts, not only because such efforts are required but also because it is the right technical thing to do.

#### CONCLUSIONS RELATED TO THE REVIEW QUESTIONS

The conclusions presented below were developed in response to each of the seven guiding questions established for this review. The questions are presented in the discussion section later in this letter.

- The ERT believes that the statement of project objectives and goals for the WAG 10 modeling effort would be more useful if they were sharpened to convey more clearly and directly to all stakeholders what the project expects to accomplish as an outcome. As currently stated, project objectives are a mixture of tasks to be performed and expected outcomes.
- 2. The ERT endorses the general technical approach being used to develop the WAG 10 site-wide groundwater model. The approach is consistent with that used in other similar projects and has the necessary components to result in a technically defensible model. The details of how to assure data quality, perform calibrations, and assess uncertainties have not yet been specified but must be included in the Work Plan. The technical and functional requirements for the numerical model must still be defined.

Mr. Erick R. Neher August 14, 2004 Page 6 of 23

- 3. The draft WAG 10 Work Plan presents a good overview of how the WAG 10 groundwater model is to be integrated with modeling results from the other WAGs, specifically WAGs 3 and 7. The proposed integration approach is not only appropriate but it is also a necessary requirement for success of the model. However, the draft Work Plan currently does not do a good job of describing how contaminant transport in the vadose zone and from the vadose zone to the groundwater (other than the K<sub>d</sub> approach) will be handled. (Apparently, other WAGs use different vadose zone models, and possibly different parameter values, in their models.) In addition, how the WAG 10 fate and transport model will integrate with the USGS flow model was not clear from the documents and presentations.
- 4. The WAG 10 project team seems fully aware of the various calibration challenges in model development that arise from the many current uncertainties in the groundwater and contaminant system to be modeled.
- 5. Although the need for one or more contaminant transport models was quite evident from the review meeting, there is currently insufficient discussion of this issue in the draft Work Plan. Few details of a planned transport model were presented. Thus, the ERT is not yet in a good position to advise and critique the plans for a site-wide contaminant transport plan.
- 6. The lessons learned from the experiences at Hanford to develop a site-wide fate and transport model can be helpful to the WAG 10 effort at the INEEL. Many of the circumstances are relevant, and the lessons learned can provide useful insight.
- 7. The WAG 10 modeling group clearly understands that there are significant data gaps, particularly with respect to the geologic framework, variability of hydraulic parameters, uneven distribution of data across the site, and sparseness of chemical data. The model development and testing efforts can provide a useful guide for additional data collection activities and for prioritizing these activities. The ERT suggests that the need for additional data should be continually re-evaluated based on modeling results. The same applies to acquisition priority, but all of this needs to be done in the context of available resources.

#### RECOMMENDATIONS RELATED TO THE REVIEW QUESTIONS

The recommendations presented below were developed in response to each of the seven guiding questions established for this review. The questions are presented in the discussion section later in this letter.

Mr. Erick R. Neher August 14, 2004 Page 7 of 23

- 1. The WAG 10 modeling team should clearly define either an overarching goal or a series of goals for the modeling effort that indicates what the project is expected to accomplish as an outcome.
  - a. Suggested language to consider for the overall project goal could include the following: "Develop a site-wide flow and transport model that can be used as a performance assessment tool to evaluate short-term and long-term remedial strategies for the aquifer and that can provide a credible estimate of cumulative risk over relevant future time frames from all contaminant sources at the INEEL".
  - b. The WAG 10 project team should also include in the Work Plan a discussion of the definition of criteria to be used to evaluate the predictive accuracy of the flow and transport model. Section 7.3 is identified as the section to address these questions in the Work Plan. The ERT urges the project team to extend this discussion beyond a typical statistical presentation, to address the broader question of defining "success" for the model capabilities.
- 2. The final Work Plan should define the technical and functional requirements and selection criteria for the ultimate model that is to be developed prior to making a determination of specific numerical codes.
  - a. To the extent reasonable, the chemical data acquired by the different groups over time for different purposes should be reconciled in terms of the flow system. An assessment should be prepared that explains the data as well as possible and considers what additional information will be required to provide a baseline set of data to be used in transport calibration and sensitivity studies.
  - b. The WAG 10 modeling group should focus on the groundwater flow model as a separately defensible tool, recognizing that it will have its own uncertainty and applications. The transport model should be considered as an extension of the flow model with options for different scales, codes, and transport mechanisms.
- 3. Efforts to improve integration of the WAG 10 flow model with the flow model activities of the USGS should be continued. This could include a documented assessment of the differences between the two models in terms of flow parameters, boundary conditions, aquifer parameters, and resulting outcomes.
  - a. In view of the importance of integrating the outcomes (fluxes and species concentrations) from vadose zone models used by other WAGs into the WAG 10 groundwater model, a review should be initiated of all presently used vadose zone models by one or more external review panels. This may clarify potential

Mr. Erick R. Neher August 14, 2004 Page 8 of 23

differences (including degree of conservativeness) in transport to the groundwater obtained with different vadose zone models.

- b. All regulatory and other stakeholder groups interested in flow and transport modeling at the INEEL should be kept informed about the WAG 10 groundwater modeling activities. E-mail-based news briefs that are sent to modelers, stakeholders and interested parties at regular time intervals, could do this. The news briefs could include contributions from many parties but should be the responsibility of WAG 10 to produce.
- 4. A methodology for the uncertainty analysis of model input parameters should be developed based on the four step process suggested, namely: 1) identification of all uncertainties related to model input parameters, 2) prioritization of these uncertainties with respect to the sensitivity of model output to these uncertainties, 3) sensitivity analysis to confirm the ranking of the prioritization of the uncertainties, and 4) communication of the uncertainties with respect to the results of the model output. The scope of the uncertainty analysis should be based in part on the agreed upon uses of the site-wide model and the level of accuracy of model outputs acceptable to regulators and other stakeholders.
- 5. A detailed work plan should be developed to arrive at one or more contaminant transport models. The ERT does not recommend development of a comprehensive new transport model that incorporates all issues that need to be dealt with at the INEEL, now and in the future. Instead, we recommend the use or adaptation of one or more existing transport models having various degrees of sophistication that can be used for a variety of needs.
- 6. The WAG 10 modeling group should make contact with their counterparts at Hanford who are involved in the development and use of a site-wide fate and transport model. The objective would be to maximize the value of applying the lessons learned at Hanford to the efforts now underway at the INEEL.
- 7. The final Work Plan needs to emphasize that, where possible within available resources, the data gaps will be filled as modeling progresses. Some data needs cannot be optimized until the model is actually used in the evaluation process.
  - a. The priorities associated with further data acquisition should be continually reevaluated to focus resources and accelerate the ability to perform calibration, sensitivity analysis, and reduction of uncertainty.

Mr. Erick R. Neher August 14, 2004 Page 9 of 23

- b. The review of data quality should be included where possible in the evaluation of data gaps, especially chemical data, so sufficient time is allowed to obtain the chemical data needed to test the transport model.
- c. The final Work Plan should elaborate on the options for simulating transport beyond the use of a K<sub>d</sub>. Other chemical processes are potentially of importance, such as solubility and precipitation.

#### RESPONSES TO INDIVIDUAL REVIEW QUESTIONS

The ERT's response to each of the seven guiding review questions is presented below:

### 1. Are the WAG 10 site-wide groundwater modeling project's objectives clear and obtainable?

Based on documents provided to the ERT and presentations during the review meeting, the objectives of the WAG 10 modeling project were defined as follows:

- a. Document recent advances in aquifer understanding.
- b. Synthesize and integrate knowledge into one comprehensive aquifer model.
- c. Communicate water and contaminant movement beneath the INEEL to a wide range of audiences.
- d. Provide a basis for the prediction of cumulative risk from all contaminant sources at the INEEL.

Additionally, a number of additional near-term and long-term objectives were presented in documents provided to the ERT, (i.e., see pages 2,3 of WAG 10 Flow and Transport Model Work Plan Objectives).

While the ERT strongly endorses the development of the WAG 10 site-wide flow and transport model, the project could benefit from a succinct, consistent statement of its objectives. There is the potential for some confusion regarding the goals, objectives and purposes of the modeling effort as currently contained in the several documents and/or handouts provided to the ERT. On one hand, development of the model is a required component of the OU 10-08 RI/FS effort, which can be defined as developing the ability to conduct "a comprehensive evaluation of impacts from the operation of the INEEL to the underlying aquifer" (Ref: WAG 10 Flow and Transport Model Work Plan Objectives). On the other hand, there are clearly a number of other possible uses for such a model, i.e., evaluating alternative remedial actions (including no action) for the aquifer, and evaluating long-term stewardship strategies as these may impact the aquifer.

Mr. Erick R. Neher August 14, 2004 Page 10 of 23

In large-scale undertakings of this nature, it is often difficult to distinguish goals and objectives from tasks that must be completed. For example, purpose "a" stated above, "Document recent advances in aquifer understanding" is better characterized as a task to be completed to achieve a larger goal, in this case, purpose "d", prediction of cumulative risk. In the Work Plan Objectives document, near-term objective "2" is described as "Identify and make recommendations for filling data gaps." Again, this is more of a task than an objective for the project.

As to whether the project objectives are believed to be obtainable, the ERT's views are a bit more complicated. The ERT is unanimous in support for this effort, and we see many benefits from successful implementation of the WAG 10 modeling project. Furthermore, we agree it is technically feasible to develop a site-wide model that can serve a number of purposes. However, it is still too early to predict whether the model will achieve the overall goal of predicting cumulative risk to hypothetical receptors at a level of accuracy that will be acceptable to regulators and other stakeholders.

While the model has the potential to reach this goal, as discussed elsewhere in this letter, current uncertainties in many parameters to be incorporated in the model raise concerns about the level of accuracy that can ultimately be achieved by final risk predictions. The ERT hastens to add, however, that this type of uncertainty is present at all contaminated sites where residual contamination is expected to remain for long periods of time, e.g., centuries. Cumulative risk over long time frames can only be evaluated using models, and models are inherently subject to short-term and long-term uncertainties that limit the accuracy of predictions.

In the ERT's experiences, there is no easy solution to this dilemma, except to recognize it and strive to minimize its effect. The WAG 10 project team should address this issue in the Work Plan by discussing in some depth the criteria to be used to define a "successful" model. Is a model that "bounds" the possible cumulative risk outcomes acceptable to all parties? What level of calibration accuracy is needed from the model to provide sufficient credibility for long-term predictions, i.e., over centuries? There are many other such questions, and we urge the project team to address as many as can be generated by parties impacted by the outcome of the modeling efforts.

### 2. Is the technical approach for a site-wide groundwater model defensible?

Yes, based on the review, the ERT believes that the broadly outlined approach being taken by the WAG 10 groundwater modeling team to creating a site-wide ground water model is technically sound at this time and is relying on generally accepted model development steps.

Mr. Erick R. Neher August 14, 2004 Page 11 of 23

From our experience, development of numerical fate and transport models in a complex system like that at the INEEL is complicated. History shows that successful development of a model takes place in sequential steps, whereas necessary data qualification and additional site characterization efforts take place in parallel. In general, the process applicable to the INEEL can be summarized as follows:

#### Sequential Steps

- The objectives and expectations of a model are stated.
- · A site-wide conceptual model is developed
- A 2-dimensional numerical model for flow is selected initially.
- The model is expanded to include 3-dimensional flow.
- · Contaminant transport requirements are matched to a numerical capability.
- Risk assessment is then initiated.

#### Parallel Activities

- Available data is quality assured.
- Data gaps are analyzed.
- Calibration/Sensitivity/Uncertainty analyses are undertaken.
- Interfacing with other WAGs for source terms/inventory/simulation needs begins.

The Work Plan being prepared by the WAG 10 modeling team will describe the procedural details for testing, calibrating, and evaluating the model at each developmental stage. The most sensitive parameters appear to have been initially identified for evaluation, e.g. geologic framework, hydraulic parameters, boundaries, etc. As the Work Plan is executed and the model to be used takes shape, the ERT believes it will be essential to its ultimate credibility that a peer review by individuals experienced in both flow and transport modeling be conducted of the progress and results.

At this point, only a few additional comments are appropriate regarding the technical approach to be described in the Work Plan:

- The Work Plan should present the method and criteria that will be used for model selection, based for example, on site needs, resources, personnel capability, expansion capability, grid flexibility, efficiency, etc. However, a specific model should not be specified. The selection of a numerical model can be done after the selection criteria are made clear and accepted.
- The Work Plan should provide for early development of a unified and consistent
  interpretation of the geochemical data that will be used. The ERT believes this
  will not only be advantageous but is imperative. Numerous geochemical studies
  have been conducted at the site on a regional and local scale. The ERT observed

Mr. Erick R. Neher August 14, 2004 Page 12 of 23

that some published geochemical data appear to be contradictory, and further, some do not seem supportable by prevailing understanding of the flow system. The geochemical data that will ultimately be used in the WAG 10 site-wide model will be an important independent constraint on the modeling effort and will be required to successfully accomplish the necessary transport calibrations and provide defensible risk simulations.

• The Work Plan should clearly differentiate development of the flow modeling capability from the transport modeling activities. Our concern is that whereas a site-wide flow model may, for example, have an extensive geographic footprint, large or variable scale, variable time steps, and 3-D or pseudo 3-D structure, the transport model may require different scales, dimensionality, etc. The transport simulations can also utilize a variety of approaches, e.g., particle tracking, dispersion only, single contaminant or multi-component reactive transport. The unifying factor will be the underlying description of flow. The transport simulations should be designed to accommodate the properties of the contaminant.

## 3. <u>Is the integration approach appropriate for other facility/WAG models (and USGS)?</u>

Conceptual groundwater models generally describe the system being modeled. This includes boundary conditions, and major inputs into the groundwater system. At the INEEL, the individual WAG's are the main potential sources of groundwater contamination, and therefore, any groundwater conceptual model of the site, and its numerical equivalent, must account for all possible inputs from the WAG's.

The approach being taken in the WAG 10 Work Plan is to invite technical staff from other WAG's (primarily 3 and 7) to participate in the WAG 10 groundwater modeling effort. The ERT believes this is a sound management approach that allows for close cooperation between the WAG 10 modeling team, and the previous and on-going work being done by the WAG 3 and WAG 7 technical staffs. It is also a bottom-up approach,

Such cooperation becomes even more important when contaminant transport is made part of the flow model. However, the ERT believes the planned quarterly meetings that will be held of INEEL modelers may not be frequent enough. In terms of site-wide model development, much can be done in a quarter, and all active modelers on-site should be informed about model development activity more frequently than every three months.

To fully integrate contaminant transport into the WAG 10 site-wide groundwater model, the contaminant fluxes, species and rates of flow must be well known for each site that is

Mr. Erick R. Neher August 14, 2004 Page 13 of 23

releasing contaminants from the vadose zone to the groundwater underneath. For many sites, these fluxes are not well known, and have to be estimated using vadose zone models. Vadose zone transport models are available but have seldom been calibrated for all contaminants at the INEEL. This adds a great deal of uncertainty to the input data (contaminant fluxes) that the WAG 10 modelers need for their groundwater model and makes it imperative that there be close coordination between WAG 10 modelers, and the vadose zone modelers associated with WAG 1, 3 and 7, and others. Such coordination is practiced right now but is not guaranteed in the future when circumstances could change.

The WAG's use different models, and possibly different values of important parameters such as K<sub>d</sub>, for predicting transport through the vadose zone at WAG's 1, 3 and 7. While this may be justified on some basis for individual WAGs, such practice could cause confusion and uncertainty when these vadose zone models, or the results from the vadose zone models, are integrated into a site-wide groundwater model.

The information presented during the review meeting and by the review documents was not clear about integrating INEEL efforts with those of the USGS. There seemed to be general agreement that groundwater model parameters for the WAG 10 and USGS models should be similar, but it was also clear that differences in the flow models of WAG 10 and USGS would persist. Such differences are not necessarily bad, as they may lead to more critical evaluations of the two models, their underlying structure and the input data used for each model. Yet, when these two models are used as decision tools, or for communication with stakeholders, it would be desirable for differences in outcome to be resolved and minimized. It was not clear to the ERT how this was going to be accomplished, but it is an issue that needs to be addressed, sooner, rather than later.

# 4. Any suggestions on an approach for setting bounds on uncertainty and uncertainty analysis?

During the review meeting, the ERT was provided with a preliminary discussion of modeling uncertainty and calibration issues by Dr. James McCarthy (see Attachment B, Review Meeting Agenda). The primary uses for the WAG 10 model were identified as: a) predictions of regional and cumulative risks, b) accurate interpretation of data, and c) identification of data gaps. Parameters were identified that would be used in model sensitivity analyses and uncertainty analyses. Thus, the WAG 10 project team seems fully aware of various calibration challenges in model development, including, but not limited to, the following: a) non-uniform distribution of monitoring wells, b) limited characterization of source terms, c) flow in fractured rock and scaling problems, if fractured rock systems are modeled with "equivalent porous media."

Mr. Erick R. Neher August 14, 2004 Page 14 of 23

Some other calibration issues that were not listed but were mentioned during discussions include: a) lack of any vertical profiling of hydraulic properties or contaminant concentrations, b) limited time frame over which hydraulic and contaminant concentration values have been measured, c) accounting for preferential pathways, d) non-equilibrium adsorption phenomena, and e) quantification of biogeochemical processes that may impact fate and transport of chemicals of concern.

The project team is in the early stages of addressing uncertainty issues, and thus, this question essentially asks for guidance from the ERT. The following discussion summarizes the ERT's views on addressing this issue:

- Uncertainty analysis for the flow and transport model should consist of at least several steps, namely: 1) identification of all uncertainties related to model input parameters, 2) prioritization of these uncertainties with respect to the sensitivity of model output to these uncertainties, 3) sensitivity analysis to confirm the ranking of the prioritization of the uncertainties, and 4) communication of the uncertainties with respect to the results of the model output. The Work Plan must establish the appropriate processes for conducting these steps, including the methodology for each of the steps. In addition, it should include an internal and external peer review process to assure adequacy of the overall process, and a methodology for incorporating stakeholder input.
- The ERT believes that the scope of the uncertainty analysis to be developed should be based in part on the agreed upon uses of the site-wide model and the level of accuracy of model outputs acceptable to regulators and other stakeholders. For example, the estimation of cumulative risks from all sources of contamination at the INEEL, including presumably both known and suspected sources, will result in specific risk calculations with a potential uncertainty of undetermined magnitude. The acceptable level of uncertainty in the final results or model outputs will, in turn, impact the level of uncertainty that is acceptable for individual model parameter inputs. In this context, it would not be appropriate for the ERT to provide a definition of "acceptable" given the need for discussions and consensus on this issue within the project team, INEEL management, and relevant stakeholders, including regulatory bodies.
- An example of this process is uncertainty analysis for hydraulic conductivity of
  the saturated zones in the modeling domain. As noted during the review meeting,
  measured hydraulic conductivities for the INEEL range over at least six orders of
  magnitude. Over 114 pumping tests have been completed to estimate the
  hydraulic conductivities across the Site. Such a wide range of uncertainty raises
  serious concerns on the ultimate accuracy of any large-scale model. However, by

Mr. Erick R. Neher August 14, 2004 Page 15 of 23

appropriate selection of stratigraphic zones, and identification of major preferential pathways in the aquifer, the range of values of the hydraulic conductivity should be better constrained, allowing for greater confidence in any fate and transport estimates generated by the site-wide model.

## 5. Any suggestions on an approach to creating flexibility in the modeling tool so it can be useful to other issues (i.e., NEPA, D,D&D, new facility siting)?

The ERT believes it would be highly desirable to create a groundwater modeling tool that could be used for many modeling tasks, including tasks that are not defined today. In theory, such a tool can do many things for many people. However, there are many examples where efforts to create a universal modeling tool have failed due to the complexity of the problems involved, the need for very fast computers with large memories, and the enormity of the programming task.

The WAG 10 groundwater model Work Plan is a modest and practical effort. It will start using a 2-dimensional model such as MODFLOW with variable thickness designed to model groundwater flow at the site. This model is quite flexible, and allows for modeling smaller scale local issues, as well as larger scale problems. By using a GMS-interface, domain boundaries, heterogeneities, point sources, sinks etc. can easily be introduced. Execution times for running the model are relatively short, and therefore, many runs can be made to test a large variety of hypotheses. The model can also be expanded to two or more layers, which might better describe the physical groundwater system at the site. However, using many layers may not be practical, and not realistic in view of the lack of detailed knowledge about the geophysical system at the site.

Because of its relative ease of use, and fast run times, a model such as MODFLOW might be well suited for outreach and education and communication with stakeholders. Versions of this model could also be used for modeling the effects of siting new facilities. This would especially be useful if such facilities would require significant quantities of water for cooling or for other purposes.

However, the current draft WAG 10 Work Plan does not mention much about modeling contaminant transport. From the discussions and presentations at the review meeting, it is quite obvious that contaminant transport modeling is a major goal of the WAG 10 groundwater modeling effort. In as much as a model such as MODFLOW was not designed for modeling contaminant transport, a separate 3-D finite difference or finite element model will have to be used. There are several such models available from established companies, as well as from nearly all of the other national laboratories. It should be possible to adapt one or more of these models for INEEL needs.

Mr. Erick R. Neher August 14, 2004 Page 16 of 23

Initially transport could be modeled using a K<sub>d</sub>-type approach, but at later stages a more complete a model coupling water flow with a multi-species contaminant model may be needed. The Work Plan and presentations were not very clear as to what the present thinking is on developing one or more of these transport models. Because of the complexity of contaminant flow through a poorly defined aquifer, a staged approach may be best, i.e. first a K<sub>d</sub>-type model, and later, a more complete model. This has the added benefit of providing greater flexibility and use, and results will be available sooner. For example, a K<sub>d</sub>-type approach may be good enough for simulating and predicting contaminant plume development over time.

# 6. What were some of the relevant lessons learned from the Groundwater/Vadose Zone Integration Project at Hanford and other site integration efforts?

Based on our collective experience at Hanford, as well as our individual experience at other DOE sites, the ERT offers several lessons learned that could benefit the current WAG 10 undertaking at the INEEL:

- a. It is critical for every major site in the DOE complex to have a technically defensible site-wide groundwater fate and transport model. This provides the basis for establishing a performance assessment capability that can meet regulatory requirements and achieve broader stakeholder acceptance regarding the impacts of site operations on regional groundwater.
- b. Development of an integrated groundwater model is a challenging but doable technical task. Progress is greatly facilitated by an atmosphere that eliminates "stovepipes" and encourages free exchange of ideas among people from the various disciplines required.
- c. Because developing an "integrated view" of the groundwater often involves some cultural adjustment to past practices and procedures, progress is also greatly facilitated by having meaningful periodic support and involvement provided by senior-level management from both the contractor and DOE sides. Success with the cultural change process requires high-level "champions."
- d. Among the key project activities that are critical to promoting stakeholder and regulatory confidence in the model and its results are: operating in a transparent fashion, involving stakeholders in the project on a continuing basis, and having periodic external merit and peer review of the progress being made.
- e. The scope of the modeling effort should be kept technically reasonable and focused on reducing key unknowns and uncertainties. The scope should not be

Mr. Erick R. Neher August 14, 2004 Page 17 of 23

allowed to become overly ambitious. Otherwise, useful results will not be produced in a reasonable period of time.

f. The benefits of developing an integrated view of the groundwater at a major DOE site include: improved ability to make cost-effective remedial and closure decisions, improved ability to communicate with regulators, stakeholders and the public, more effective field data gathering efforts, and greater ability to focus supporting research and science and technology projects so they yield relevant information on a timely basis.

#### 7. Can you provide any evaluation of data gaps for the site-wide modeling effort?

It is clear to the ERT that the WAG 10 modeling group is sensitive to the issue of identifying and filling data gaps for the site-wide modeling effort. The issue is identified specifically in the draft Work Plan, and the presentation by Mr. Tom Wood during the review meeting clearly indicted that identification of "data gaps" was well underway. The ERT applauds this effort and offers the following suggestions for supporting the description of this issue in the final Work Plan:

- a. Define the Process as Open-Ended Some data needs have already been identified that are important if not critical to clarifying the conceptual model and calibrating the numerical flow model. Other data needs cannot be firmly determined until uncertainty analysis and preliminary simulations are made. Therefore, the process of filling the gaps cannot be done "up front" but will extend over the life of the project. Resources will be needed over time to progressively and deliberately acquire new data, especially as modeling progresses and optimum locations and data types are identified. The Work Plan should contain appropriate statements regarding the effort to progressively reduce uncertainty by optimizing acquisition of new data following incorporation of the latest information.
- b. Conclude Background Sections of the Work Plan with a Summary Statement of Key Uncertainties The Work Plan will summarize what is known about the relevant physical system in terms of the three key geoscience disciplines that impact modeling of groundwater: (1) geologic setting, (2) hydrogeology, and (3) geochemistry. The history of data collection shows that data have been unevenly collected across the site and obtained for purposes often unrelated to groundwater modeling studies. It would be beneficial in the Work Plan to add a summary section to each of the three geoscience sub-chapters that identifies key areas of uncertainty related to that discipline. A "key uncertainty" summary section for

Mr. Erick R. Neher August 14, 2004 Page 18 of 23

each geoscience discipline will place the discussion of background knowledge into a context of a baseline for the discussion of data gaps in another chapter.

- Chapter 6 of the draft Work Plan will c. Create a Dynamic Priority Structure identify the data acquisition plan. Additional data for groundwater modeling are necessary, but the effort to fill data gaps will never yield a complete data set. The Work Plan must convey how the data acquisition process is to be prioritized. The Wag 10 modeling team has created an initial list of data needs, some of which were indicated to the ERT at the meeting. Further, within the Work Plan many of the data needs will be defined explicitly as data gaps, with a proposed solution to obtain the additional data required for the groundwater model. This process will be difficult, so the Work Plan should address the procedure for giving priority to the most critical needs. The criteria that the WAG 10 modeling group will use to develop the priority list were not presented at the review meeting. The Work Plan should define the criteria for selecting the data needs, and describe the method for creating priority among the many potential data acquisition activities, among different geoscience disciplines. The Plan should also identify a mechanism for re-evaluation of the priority of data acquisition as new data are obtained.
- d. Provide Project Detail Beyond the Groundwater Flow Model Creating consistency across the site in modeling groundwater flow is essential; but the success of the model as a risk assessment tool will require substantial attention to developing confidence in the transport calculation. The WAG 10 modeling team has identified many of the weakness of previous modeling efforts and has begun to compile a list of what new data will be required to improve these conceptual and numerical simulations. The transport of tritium, organics and reactive solute will be the drivers for the risk calculation. Significant effort will be required to select the appropriate scale of modeling, define and quantify the processes of reaction, and select the numerical methods needed just to calibrate the transport model and evaluate the representativeness of the simulation.

There are data needs in this arena that may require external modeling and experimental work not generally considered as data acquisition. For example, in both the draft Work Plan outline and in the presented material, only the  $K_d$  has been discussed as the retarding factor in transport. Solubility of solvents and some radionuclides will certainly be a factor, and volatilization may be a significant complicating factor to the interpretation of solute distribution. Regarding the process of sorption/desorption, the  $K_d$  values may actually not be "constants" but may be variable along the flow path based on rock type, mineral surface weathering conditions, and aqueous complexation with ligands like bicarbonate, carbonate and sulfate in solution.

Mr. Erick R. Neher August 14, 2004 Page 19 of 23

A common data requirement in transport modeling is for the chemical datasets to be reviewed for quality. It was not clear during the review meeting whether the existing chemical database had gone through an adequate Quality Assurance process. Procedures and methods should be identified and clearly defined in the Work Plan that will provide the needed confidence in the chemical data, constants, and numerical procedures.

#### **DOCUMENTS REVIEWED (in priority order)**

WAG 10 OU 10-08 Site-Wide Groundwater Model Work Plan, draft annotated outline, as of May 19, 2004.

Arnett, R., and Smith, R., 2001, WAG 10 Groundwater Modeling Strategy and Conceptual Model, INEEL/EXT-01-00768, Revision B (draft)

BBWI, 2003, INEEL Subregional Conceptual Model Report Volume 1 – Summary of Existing Knowledge of Natural and Anthropogenic Influences Governing Subsurface Contaminant Transport in the INEEL Subregion of the Eastern Snake River Plain, INEEL/EXT-02-00987

Smith, R. P., 2002, Aquifer Thickness Assessment for Use in WAG 10, OU 10-08 Groundwater Modeling Activities, BBWI INTERNAL REPORT, INEEL/INT-01-01458, Revision 0.

Roddy, M.S., and Koeppen, L.D., 2004, Evaluation of Aquifer Contaminants Upgradient from the Radioactive Waste Management Complex, BBWI INTERNAL REPORT, ICP/INT-04-00285.

Roback, R.C., Johnson, T.M., McLing, T.L, Murrell, M.T., Luo, S., and Ku, T., 2001, Uranium Isotopic Evidence for Groundwater Chemical Evolution and Flow Patterns in the Eastern Snake River Plain Aquifer, Idaho, GSA Bulletin, V. 113, No. 9, p. 1133-1141.

McLing, T.L, and Smith, R.W, 2001, Chemical Characteristics of Thermal Water beneath the Eastern Snake River Plain, Geological Society of America, Special Paper 353.

Johnson, T., Roback, R., McLing, T. Bullen, T., DePaolo, D., Doughty, C., Hunt, R., Smith, R., Cecil, D., 2000, Groundwater "Fast Paths" in the Snake River Plain Aquifer: Radiogenic Isotope Ratios as Natural Groundwater Tracers, Geology, V. 28, No. 10, p. 871-874.

Mr. Erick R. Neher August 14, 2004 Page 20 of 23

This concludes our comments on the review that we performed. We stand ready to amplify our comments, if necessary, and answer any additional questions that you or the WAG 10 modeling team might have.

Yours very truly,

Edgar Berkey, Ph.D., Chair

R.L. Bassett, Ph.D. Michael Kavanaugh, Ph.D. Peter Wierenga, Ph.D.

cc: Michael Graham – BBWI Michael Hodel – BBWI Tom Wood – BBWI

Attachment A: Bio-sketches of the External Review Team

Attachment B: Review Meeting Agenda

Mr. Erick R. Neher August 14, 2004 Page 21 of 23

#### ATTACHMENT A

#### BIO-SKETCHES OF THE EXTERNAL REVIEW TEAM

#### **Edgar Berkey**

Dr. Berkey is a senior consultant to the Department of Energy (DOE), Environmental Protection Agency (EPA), and industry and a vice president of Concurrent Technologies Corporation with over 35 years of experience. He holds a B.S. in Chemical Engineering from Stanford University and a Ph.D. in Nuclear Science and Engineering from Cornell University. He was a member of DOE's Environmental Management Advisory Board (EMAB) for six years, EPA's Science Advisory Board for four years, and chairman of the Groundwater/Vadose Zone Expert Panel at Hanford for three years. He currently chairs the Energy and Environmental Technology Directorate Review Committee for the Idaho National Engineering and Environmental Laboratory (INEEL) and is also a member of the Laboratory Advisory Committee, as well as the Environmental Technology Directorate Review Committee of the Pacific Northwest National Laboratory (PNNL). In addition, Dr. Berkey is a member and former chairman of the Environmental Advisory Committee for DOE's Savannah River Site (SRS). Dr. Berkey has been an adjunct Associate Professor of Environmental Engineering at the University of Pittsburgh and Co-Director of the EPA-funded Groundwater Remediation Technologies Analysis Center.

#### R.L. Bassett

Dr. Bassett is president of Geochemical Technologies Corp. He was a Professor in the Department of Hydrology and Water Resources at the University of Arizona for 14 years, where he continues as an adjunct Professor and directs the isotope laboratory. He holds a B.S. in Geology from Baylor University, a M.S. in Geochemistry from Texas Tech University, and a Ph.D. in Environmental Geochemistry from Stanford University. He has been principal investigator for numerous field and laboratory research projects such as DOE Siting Studies in Arizona. He has published extensively in peer-reviewed journals on issues related to radioactive waste geochemistry, ground water geochemistry, siting, isotopic geochemistry, contaminant migration and transport. He was a Darcy Distinguished Lecturer and an Associate Editor for the journals of Water Resources Research, Ground Water, and Applied Geochemistry. He has served on numerous review panels and boards, such as the University of Waterloo Centre for Groundwater Research Advisory Committee; National Academy of Sciences Committee on Low Level Radioactive Waste; Argonne National Laboratory Radioactive Waste Review Panel; Board of Directors of the National Ground Water Association, Association of Ground Water Scientists and Engineers; and the Hanford Ground Water/Vadose Zone Expert Panel.

Mr. Erick R. Neher August 14, 2004 Page 22 of 23

#### Michael A. Kavanaugh

Dr. Kavanaugh is Vice President and the National Science and Technology Leader for Malcolm Pirnie, Inc. He has over 30 years of consulting experience as a chemical and environmental engineer to private and public sector clients in the U.S., Western Europe, and the World Bank. His areas of expertise include hazardous waste management, soil and groundwater remediation, strategic environmental management, risk analysis, water quality with an emphasis on emerging contaminants, water treatment, water reuse. industrial and municipal wastewater treatment and technology evaluations including patent reviews. He has served on many advisory panels at DOE facilities, including the Hanford Groundwater/Vadose Zone Expert Panel, and external reviews at the Oak Ridge National Laboratory, the INEEL, Lawrence Livermore National Laboratory, and Los Alamos National Laboratory. Dr. Kavanaugh chaired the Board on Radioactive Waste Management of the National Research Council from 1998 to 2000. He has a B.S. and a M.S. in Chemical Engineering from Stanford University and the UC Berkeley, respectively, and a PhD in Civil/Environmental Engineering from UC Berkeley. He is a registered professional engineer in several states, a Diplomate of the American Academy of Environmental Engineers, a Consulting Professor in the Environmental Engineering Department of Stanford University, and was elected to the National Academy of Engineering in 1998.

#### Peter J. Wierenga

Dr. Wierenga obtained a master's degree from Wageningen University in the Netherlands, and a Ph.D. degree in soil physics from the University of California, Davis. He taught soil physics at New Mexico State University for 20 years, where he had an active research program in water flow and contaminant transport through the vadose zone. With funding from EPA, NRC, the State of New Mexico and others, he conducted many large field studies in cooperation with colleagues at New Mexico State and New Mexico Tech. Subsequently, he became a department head at the University of Arizona and led the transformation of a traditional soils department to a diversified Environmental Sciences Department. For the last 5 years, Dr. Wierenga has been Director of the Arizona Water Resources Research Center. At Arizona, he has performed field experiments on vadose zone processes with colleagues from Hydrology and other departments. He was a member of the Hanford Ground Water/Vadose Zone Expert Panel and has published over 200 papers and reports, including over 100 as refereed journal articles. He is a fellow of the American Geophysical Union, American Association for the Advancement of Science, and the SSSA, as well as a highly cited author.

Mr. Erick R. Neher August 14, 2004 Page 23 of 23

#### **ATTACHMENT B**

#### WAG 10 GROUNDWATER MODELING REVIEW MEETING AGENDA

#### May 19, 2004

8:00 am Welcome and Introductions Erick Neher

Meeting Objectives and Agenda

Background on Balance of INEEL Michael Graham

Cleanup Project Objectives

Modeling Objectives and Integration Approach Tom Wood

Snake River Plain Aquifer Hydrogeology Brennan Orr

Aguifer Fast Flow Paths Travis McLing Swen Magnuson

Contaminant Source Terms and Vadose Zone

Transport

**INEEL Aquifer Contaminant Plumes** Mike Roddy

1:00 pm Modeling Overview and Approach Mike Rohe

Hai Huang

Modeling Uncertainty and Calibration Dr. James McCarthy

OU 10-08 Data Gaps to Support Modeling Tom Wood

Interview of 10-08 Modeling Team Review Team

5:00 pm External Review Team Deliberations

May 20, 2004

8:00 am Interview of 10-08 Modeling Team Review Team

9:30 am External Review Team Deliberations

11:00 am Outbrief to 10-08 Modeling Team Review Team

May 21, 2004

8:15 am Outbrief to DOE-ID Michael Graham

(Lisa Green and Katie Hain) Review Team

### Appendix B

Groundwater Transport Modeling Using the Response Function and Convolution Integral

# GROUNDWATER TRANSPORT MODELING USING THE RESPONSE FUNCTION AND CONVOLUTION INTEGRAL

Arthur S. Rood

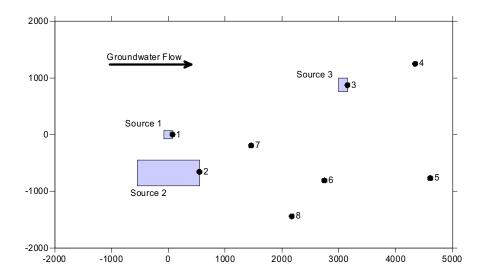
November 23, 2004

#### Introduction

Numeric models of groundwater flow and transport can be time consuming and resource-intensive to run even on modern computing systems. This is especially true if many contaminant sources and multiple contaminants are simulated. A method is proposed to reduce the computational requirements for simulation of multiple contaminants and multiple contaminant sources in an aquifer system. This approach is based on the response function discussion in Gorelick (1983). It uses the convolution integral coupled with source-receptor response functions and contaminant fluxes to the aquifer to estimate groundwater concentrations at selected receptor locations in the groundwater modeling domain. The approach retains most of the complexity of the flow and transport modeling performed using numerical models, although some simplifying assumptions are necessary.

### Methodology

Consider the model domain illustrated in Figure 1. Within the domain there are three sources and within each source there are multiple contaminants. Each source has a "footprint" where contaminants from the vadose zone enter the aquifer. Within the model domain there are eight receptor locations. These locations can represent existing wells, future wells, and points of interest in the aquifer. For example, receptor number 1, 2, and 3 may not represent actual wells, but points in the aquifer where the maximum contaminant concentration in groundwater from an individual source is achieved.



**Figure 1.** Hypothetical aquifer domain for demonstration of the convolution integral. The systems has three contaminant sources and eight receptor locations.

The breakthrough curve at each receptor to a unit mass input from each source is the response function. The response functions for each of the three sources at the eight receptor locations are illustrated in Figure 2. Note that for Source 3, only three receptors are shown because the remaining receptors lie up gradient from Source 3 and are therefore unaffected by releases from the source. The response function is determined using the groundwater flow and transport model and represents the concentration in the aquifer as a function of time for a conservative, non-decaying, non-sorbing tracer of unit mass released to the aquifer over the source footprint at time zero.

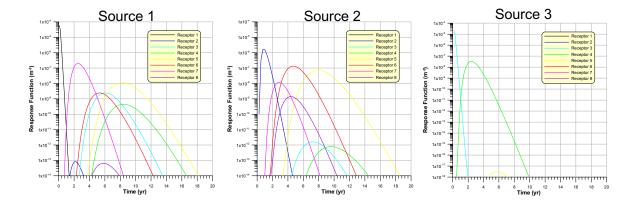


Figure 2. Response function for each receptor-source pair.

The contaminant loading rates to the aquifer from each source are illustrated in Figure 3. These graphs represent the contaminant flux to the aquifer as a function of time for a single contaminant. However, multiple contaminants with varying sorption and decay properties can also simulated by developing source loading rates for each contaminant.

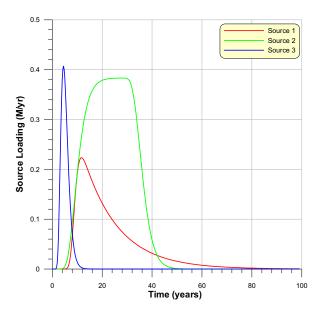


Figure 3. Source loading rates for each of the three sources.

The contaminant concentration in the aquifer at a given receptor location then represents the convolution of the source loading rates and the response function. That is, the source loading rates can be represented by a series of individual pulses that when summed together, form a continuous function. The contaminant concentration is then given by

$$C_{i,j}(t) = \int_0^t RF_{i,j}(t-\tau)S_i(\tau)d\tau \tag{1}$$

where

 $C_{i,j}(t)$  = aquifer concentration of a contaminant at time t for source i and receptor j (M L<sup>-3</sup>)

 $RF_{i,j}(t-\tau)$  = response function for source *i* and receptor *j* at time  $t-\tau(L^{-3})$ 

 $S_i(\tau)$  = source loading rate for source *i* at time  $\tau$  (M T<sup>-1</sup>)

Equation (1) is valid for a non-decaying, non-sorbing contaminant. The quantity  $t - \tau$  is the "age" of the pulse. To account for the different decay and sorptive properties of a contaminant, several simplifying assumptions are made:

- Sorption is uniform throughout the aquifer
- Decay is constant throughout the aquifer
- Parent and progeny travel at the same rate in the aquifer

The aquifer concentration for a decaying and sorbing contaminant that may generate decay products in transit is given by

$$C_{i,j,k}(t) = \frac{1}{Rd_k} \int_0^t RF_{i,j} \left( \frac{t - \tau}{Rd_k} \right) S_{i,k}(\tau) DIF_k(t - \tau) d\tau$$
 (2)

where

 $C_{i,j,k}(t)$  = aquifer concentration of contaminant k at time t for source i and receptor j (M L<sup>-3</sup>)

 $RF_{i,j}(t-\tau)$  = response function for source *i* and receptor *j* at time  $t - \tau(L^{-3})$  $S_{i,k}(\tau)$  = source loading rate for contaminant *k* and source *i* at time  $\tau(M T^{-1})$ 

Rdk = the retardation factor for contaminant k (unitless)

 $DIF_k$  = decay-ingrowth factor for contaminant k at time  $t - \tau$  (unitless)

The decay-ingrowth factor is the activity of decay product k present at time  $t - \tau$  relative to the original parent activity released at time  $\tau$ . For a single decay species with no progeny, the decay ingrowth factor is simply  $\exp[-\lambda(t-\tau)]$ . For a decay product other than the parent, the decay-ingrowth factor is given by

$$DIF_{k}(t) = \frac{\lambda_{k}}{\lambda_{1}} \left[ \left( \prod_{i=1}^{k-1} \lambda_{i} \right) \sum_{i=1}^{k} \frac{e^{-\lambda_{i}t}}{\prod_{\substack{j \neq i \ j=1}}^{k} \left( \lambda_{j} - \lambda_{i} \right)} \right]$$
(3)

where

 $\lambda_1$  = decay constant for the parent (T<sup>-1</sup>)

 $\lambda_k$  = decay constant for the  $k^{\text{th}}$  progeny (T<sup>-1</sup>)

t = age of pulse (T).

The total contaminant concentration from all sources is evaluated by superposition of each source-receptor pair. That is, the contaminant concentration at a given receptor location from multiple sources is the sum of the concentration from each individual source.

$$C_{j,k}(t) = \sum_{i=1}^{n} C_{i,j,k}(t)$$
(4)

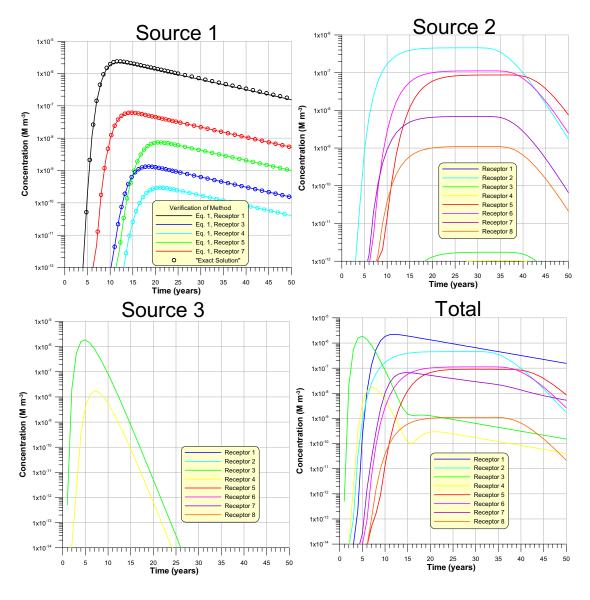
where n is the number of sources considered in the model domain.

Figure 4 illustrates the results of the aquifer domain illustrated in Figures 1–3 for a conservative non-decaying and non-sorbing contaminant. The GWSCREEN code (Rood 1999) was used to calculate the response functions and source loading rates. The GWSCREEN model combines a source release model, a one-dimensional unsaturated transport model, and a three-dimensional aquifer transport model assuming unidirectional flow in a homogeneous and isotropic aquifer of infinite lateral extent and finite thickness. The GWSCREEN model also uses the convolution integral to compute groundwater concentrations from an arbitrary source loading rate. The response function in GWSCREEN is calculated using an analytical solution to the advection dispersion equation for the aforementioned boundary conditions. The response function used in this demonstration employed the same analytical solution but was represented by a series of tabulated values. These tabulated values were read into a FORTRAN program and stored in an array. Linear interpolation was then used to derive the response function value at any point in time.

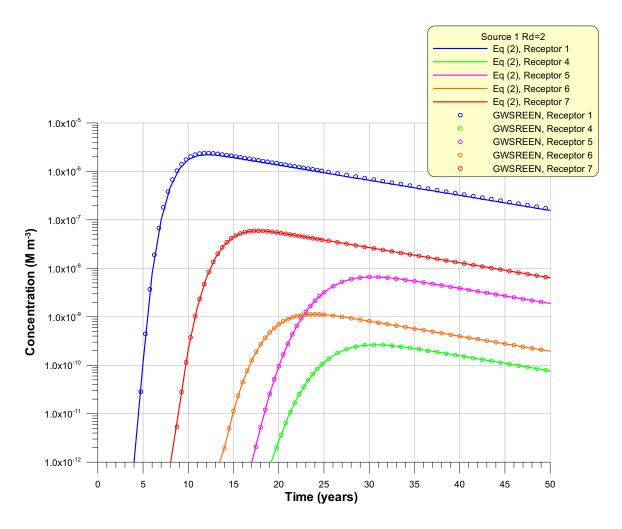
Source loading rates were also calculated using GWSCREEN, stored as tabulated values, and linearly interpolated. The GWSCREEN model was used for demonstration of the methodology, but any model, or combination of models could be used in actual practice. The graph for Source 1 includes a comparison to the "exact solution" as determined by GWSCREEN.

Figure 5 shows a comparison of concentrations at selected receptor locations for Source 1 and a contaminant having an retardation factor of 2. This figure can be compared to the graph for Source 1 in Figure 4 that represents a contaminant with a retardation factor of 1. The source loading rates were the same for both simulations, but a retardation factor of 2 in the aquifer was used in Figure 5. The solution using GWSCREEN is also shown for comparison. Qualitatively, there is very little difference between the "exact" solution determined with GWSCREEN and the response function approach discussed here.

In summary, the response function method discussed here is a viable method incorporate a relatively complex groundwater flow and transport model into an assessment framework that considers arbitrary source loading rates for numerous sources and contaminants.



**Figure 4.** Contaminant concentration as a function of time at each of receptor location for all individual sources and total as determined by Equation 4.



**Figure 5.** Contaminant concentration as a function of time for Source 1 and a contaminant having a retardation coefficient of 2. Compare with the graph for Source 1 in Figure 4.

### References

Rood, A. S., 1999. *GWSCREEN: A Semi-Analytical Model for Assessment of the Groundwater pathway from Surface or Buried Contamination, Theory and User's Manual Version 2.5.* INEEL/EXT-98-00750, Rev 1 February, Idaho National Engineering and Environmental Laboratory, Idaho Falls, Idaho.

Gorelick, S. M., 1983. "A Review of Distributed Parameter Groundwater Management Modeling Methods." *Water Resources Research*, 19(2), 305-319. April 1983.